



Assignment Description

Bioinformatics 2021/2022

Introduction

- Write a Tcl code
- You are required to practice the concepts learned throughout course

Requirements

Main Program

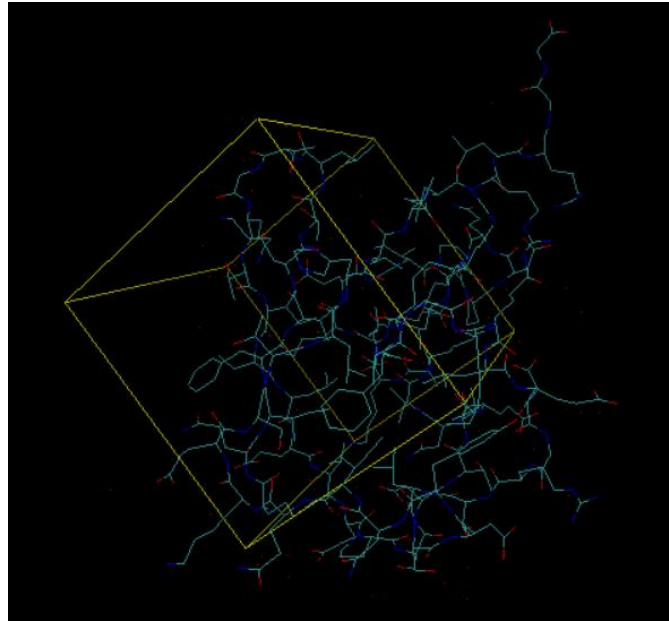
Write a Tcl program that starts with displaying a menu for the user to choose a specific action and based on his/her action start to call the appropriate answer (Task Load 20 %)

e.g.

```
Hello User, Choose your action with number from 1 to 6
1. Load File
2. Select a residue
3. Save Selection
4. Analyze
5. Process Residues
6. Align Molecules
```

Detailed Description

1. Load File (Task Load 10%)
 - 1.1. Implement a function that asks the user for the file name/path to load the file.
 - 1.2. If user entered a directory print a list with all pdb files in this directory.
 - 1.3. If user entered a file name, make sure it exists and accessible (print proper error message if not)
2. Select a residue (Task Load 20%)
 - 2.1. Implement a function which asks the user for the residue name/range.
 - 2.2. Draw a box surrounding the selected atoms.
 - 2.3. Make sure that user has already loaded a file



Output for 1ubq.pdb with residue ids selected from 1 to 10

3. Save Selection (Task Load 20%)
 - 3.1. Implement a function that saves a selection
 - 3.2. Make sure that user has already selected atoms before
 - 3.3. Ask the user for a folder/path to save data in
 - 3.4. Make sure that the path exist (print proper error message if not)
 - 3.5. Make sure user have access to save in the path (print proper error message if not)
 - 3.6. Ask user for file name
 - 3.7. Save the file as pdb
4. Analyze (Task Load 10%)
 - 4.1. Implement a function which prints all information for a selection
 - Number of atoms
 - Number of bonds
 - Number of residues
 - 4.2. Make sure that output is formatted well (Hint: Use string format)

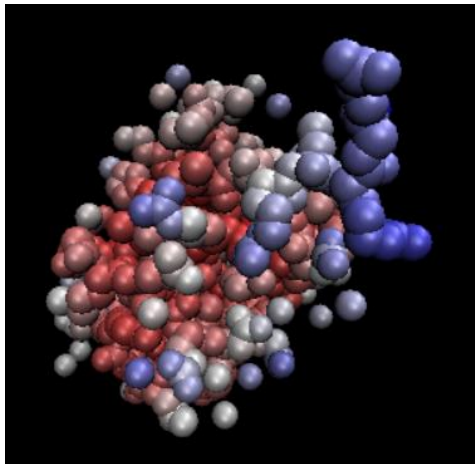
Number of atoms:	660
Number of bonds:	608
Number of residues:	134

Output for 1ubq.pdb

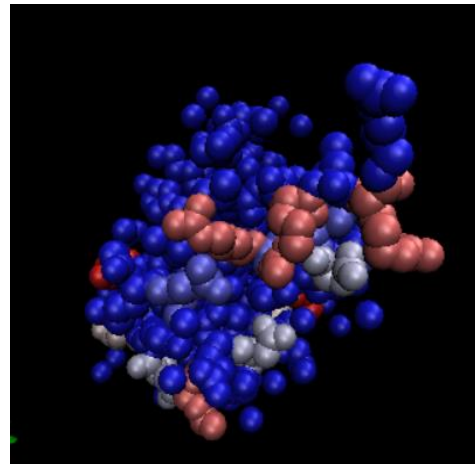


5. Process Residues (Task Load 20%)

- 5.1. Implement a function that gets all residues
- 5.2. Print number of atoms in each residue
- 5.3. Draw each residue with different color
(e.g. first residue with beta 0 second with beta 10 etc.)
- 5.4. Output formatted as in table (Hint: use format string function)



Before



After

ALA	10
ARG	44
ASN	16
ASP	40
GLN	54
GLU	54
GLY	25
HIS	10
HOH	58
ILE	56
LEU	72
LYS	63
MET	8
PHE	22
PRO	21
SER	18
THR	49
TYR	12
VAL	28

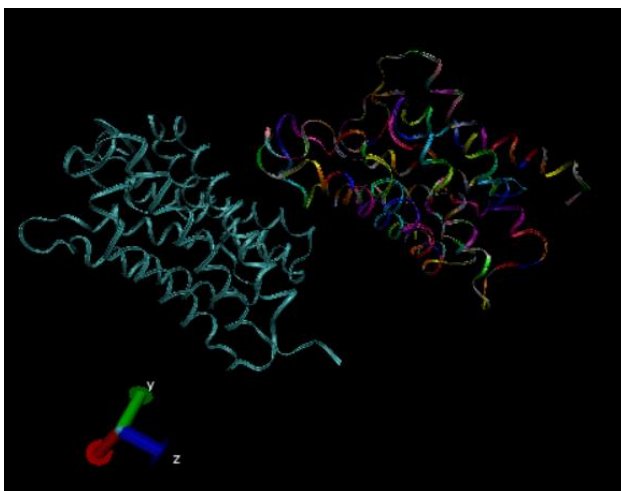
Output

Output for 1ubq.pdb

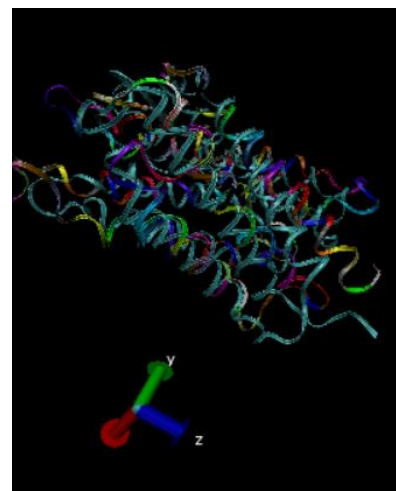
6. Align molecules (Bonus Task with Load 20%)

Implement a function that do the following functions

- 6.1. Make sure that the OpenGL menu have no drawing (clear window)
- 6.2. Ask user to enter 2 file names
- 6.3. Load files
- 6.4. Move the molecules to be aligned on top of each other



Before aligning



After aligning

Output for 1fqy.pdb and 1rc2.pdb



Assignment Policy:

- This is a group assignment of exactly 3 members
- If you submit as a group of more than/less than of 3 members, All the group members will get zero
- Assignment deadline is 13/5 at 11:59 pm
- You will put your code in file named
Assignment_firstStudentID_secondStudentID_thirdStudentID.tcl
- Submitted code must be working properly with the specified output
- All students should work and fully understand everything in the submitted solution.
- No late submission is allowed.
- Submissions will be on the blackboard. It is your duty to ensure that your submission was properly uploaded to the blackboard after you finish submitting it. If your submission was not uploaded properly while marking, you will not receive a grade for the assignment.
- No submission through e-mails.
- Failing to abide by the naming convention of the file or failing to submit the files as per the requested extension, would result in a zero for all team members.
- In case of cheating, you will get a negative grade whether you give your solution to someone, take the solution from someone/internet, or even send it to someone for any reason.
- If the team or any member didn't attend the discussion without formal excuse before the discussion time the whole team will get zero grade.